

## MM 14: Transport II: Atomic and ionic transport

Time: Monday 15:45–17:30

Location: H53

MM 14.1 Mon 15:45 H53

**Finding ultrafast diffusion in cold-rolled Nickel** — ●SIMON TRUBEL<sup>1</sup>, SERGIY DIVINSKI<sup>1</sup>, MARTIN PETERLECHNER<sup>1</sup>, CHRISTIAN SIMON<sup>1</sup>, EHUD ALMOG<sup>2</sup>, ERHARD SCHAFER<sup>3</sup>, and GERHARD WILDE<sup>1</sup> — <sup>1</sup>Institut für Materialphysik, WWU Münster — <sup>2</sup>Dep. of Materials Science Engineering, Technion, Haifa — <sup>3</sup>Physics of Nanostructured Materials, University of Vienna

Ultrafast diffusion rates have been found in a number of severely plastically deformed (SPD) materials. SPD processing produces an ultrafine grained microstructure while, at certain conditions, is able to modify grain boundaries into a specific (\*non equilibrium\*) state, at least a fraction of them. This fact was unambiguously shown for nickel of 99.6% purity deformed via ECAP or HPT [1]. At this point, an open question arises - does a critical deformation exist which would correspond to an appearance of such a characteristic state of grain boundaries?

Cold rolled Nickel of the same purity was investigated applying different deformation methods. Partial annealing of cold rolled nickel was found to open diffusion channels with characteristics alike to a porosity network. The formation of these paths was investigated via x-ray diffraction and electron microscopy in combination with calorimetric analysis. Grain boundary self-diffusion was measured applying the <sup>63</sup>Ni radioisotope and precision mechanical sectioning. The results are discussed concerning the formation conditions of grain boundaries that would act as ultrafast diffusion paths.

[1] S. V. Divinski, et al. Acta Mater., 59, 1974 (2011).

MM 14.2 Mon 16:00 H53

**Effect of precipitation on grain boundary diffusion in an Al-based alloy** — ●BENGÜ TAS KAVAKBASI<sup>1</sup>, VLADISLAV KULITCKII<sup>2</sup>, SERGIY V DIVINSKI<sup>1</sup>, and GERHARD WILDE<sup>1</sup> — <sup>1</sup>Institute of Materials Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48341 Münster, Germany — <sup>2</sup>Belgorod State University, Belgorod, 308015, Russia

Precipitation phenomena affect the kinetics of diffusion in the surrounding matrix. The present study is focused on the effect of Al<sub>3</sub>Sc precipitates on grain boundary diffusion in an Al-based AA5420 alloy (Al-4.6Mg-0.64Mn-0.2Sc-0.09Zr-0.2Ti-0.08Fe-0.02Si). Different states were prepared by combination of ECAP processing and heat treatments and the radioisotope <sup>57</sup>Co was employed as a sensitive probe of a given grain boundary state. The results suggest that Co diffusion at room temperature is intimately coupled to the precipitation behavior of Al<sub>3</sub>Sc at elevated temperatures. In fact, the Co diffusion coefficients are first decreasing with increasing precipitate size and approach a minimum at their average size of about 20 nm, which is probably related to maximal elastic stresses around the precipitates. As the precipitates grow further, the diffusion coefficients begin to increase due to a loss of coherence accompanied by a change in the chemical composition and a reduction of stresses around the precipitates.

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MM 14.3 Mon 16:15 H53

**Hydrogen sorption kinetics of titanium hydride thin films** — ●LUKAS MICHALEK, EFI HADJIXENOPHONTOS, and GUIDO SCHMITZ — University of Stuttgart, Institute for Materials Science, Heisenbergstrasse 3, 70569 Stuttgart, GERMANY

Titanium hydride has been studied a lot in the last few years because of its impressive hydrogenation kinetics. Transition metals are known to improve hydrogen (H) storage materials and act as catalysts in the diffusion process. Despite the low weight percentage of H it can take (4wt.%), it is a material in which H diffuses very easily and furthermore it's stable in air. In this work, we focus on the H-sorption behavior in thin films of thickness 50-400nm in different conditions. Pure  $\alpha$ -Ti samples were deposited by ion beam sputtering on Si substrates. Hydrogenation was studied at different temperatures (RT-300°C) at 1-10 bars of H atmosphere for different duration of time (60-600min) in order to measure the kinetic barriers at the interfaces and diffusion coefficients. Hydrogen sorption was quantified by X-ray Diffraction, TEM was used for microstructural analyses and surface analysis was studied by SEM. A pure  $\delta$ -TiH<sub>2</sub> peak appears in the XRD characterization for samples hydrogenated over 100min at 300°C and 10bars of H. Full dehydrogenation of this material is more challenging because

of the stability of the hydride. Also the substrate choice appears to play an important role. Possible reversibility of  $\delta$ -TiH<sub>2</sub> to  $\alpha$ -Ti has been studied on magnesium oxide and aluminum oxide. The observed sorption behavior at these conditions will be the focus of this work.

15 min. coffee break

MM 14.4 Mon 16:45 H53

**Descriptors of lithium-ionic conductivity from first-principles molecular dynamics** — ●LEONID KAHLE<sup>1</sup>, ARIS MARCOLONGO<sup>1</sup>, NICOLA MARZARI<sup>1</sup>, and BORIS KOZINSKY<sup>2</sup> — <sup>1</sup>Theory and Simulation of Materials (THEOS), and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland — <sup>2</sup>Robert Bosch LLC, Research and Technology Center, Cambridge, Massachusetts 02142, USA

We present a high-throughput study of lithium-ion conductivities obtained from extensive first-principles molecular dynamics simulations. Structures and trajectories are analyzed using methods and algorithms mutated from the field of computational geometry. First, we introduce a rigorous approach to discretize the volume of any arbitrary crystal structure into physically meaningful interstitial sites. Then, we illustrate how to track atoms or ions of interest through the course of a simulation and how to detect jumps between interstitial sites with high spatial and temporal resolution. This approach allows us to correlate dynamical, structural and chemical properties of sites and materials with observables such as occupation densities and jump frequencies. We will conclude with the results obtained analyzing 3300 Born-Oppenheimer molecular dynamics simulations performed on 1200 Li-containing structures at varying temperatures, with the aim of identifying critical descriptors for Li-ion transport.

MM 14.5 Mon 17:00 H53

**Transport of ions in a mixed Na<sup>+</sup>/K<sup>+</sup> ion conducting glass - electrodiffusion profiles and electrochemical interphase formation** — ●JOHANNES MARTIN<sup>1</sup>, SARAH MEHRWALD<sup>1</sup>, MARTIN SCHÄFER<sup>1</sup>, THILO KRAMER<sup>2</sup>, CHRISTIAN JOOSS<sup>2</sup>, and KARL-MICHAEL WEITZEL<sup>1</sup> — <sup>1</sup>Fachbereich Chemie, Philipps-Universität Marburg — <sup>2</sup>Institut für Materialphysik, Universität Göttingen

The competition of Na<sup>+</sup> ion versus K<sup>+</sup> ion transport in a mixed alkali borosilicate glass has been investigated by low energy bombardment induced ion transport employing Cs<sup>+</sup> ions as the foreign ion. Electrodiffusion causes the replacement of Na<sup>+</sup> and K<sup>+</sup> down to about 200 nm below the surface of the glass. Beyond this electrodiffusion front (in the direction of ion transport) K<sup>+</sup> ions accumulate to a density above the bulk concentration while Na<sup>+</sup> is further depleted towards the backward electrode. At the backward electrode only Na is electrodeposited since the electrical potential does not allow for K electrodeposition. A full simulation of the electrodiffusion profiles reveals the complete concentration dependence of the diffusion coefficients of the Na<sup>+</sup> and K<sup>+</sup> ions.

MM 14.6 Mon 17:15 H53

**The mechanism of mixed ionic and electronic transport during electro-thermal poling** — ●MARTIN SCHÄFER and KARL-MICHAEL WEITZEL — Fachbereich Chemie, Philipps-Universität Marburg

Electro-thermal poling is a technique that allows to investigate and manipulate physical properties of solid electrolytes, e.g. ion conducting glasses, in particular at the sample surface. During the poling experiment, the sample is placed between two ion blocking metal-electrodes and an electric field is applied at elevated temperatures. The charge carriers inside the sample move according to the field and give rise to an ion depletion zone below the anode. Usually, the buildup of the depletion zone is accompanied by the decay of the poling current and by the simultaneous expulsion of the field from the bulk of the sample such that eventually a strong field remains in the depletion zone solely. Here, a calculation based on a Monte-Carlo simulation is presented that describes the mechanism of electro-poling in samples with more than one mobile carrier species. The model explicitly includes the diffusion of two ion species and the electron mobility at electric field strengths beyond the breakdown field strength. The calculations show

that for certain ion mobilities, the time evolution of the potential and the current decay occur on significantly different time scales. Diffusion profiles are calculated and compared to experiments from literature. Very good agreement is reached.